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| <input type="checkbox"/> | L15 l8 and l14 | 1976 |
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| | <i>DB=USPT; PLUR=YES; OP=OR</i> | |
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FILE LAST UPDATED: 20 Apr 2004 (20040420/ED)
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=> s ((DNA#(10a)melt?)(20a)calculat?)/bi,ab 662213 DNA#/BI
526844 DNA#/AB 517963 MELT?/BI 451480 MELT?/AB 163067
CALCULAT?/BI 20861 CALCULAT?/AB

L1 12 ((DNA#(10A)MELT?)(20A)CALCULAT?)/BI,AB

=> d l1 1-12 bib ab

L1 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:671712 CAPLUS
DN 136:320824

TI ***Calculating*** sequence-dependent ***melting***
stability of duplex ***DNA*** oligomers and multiplex sequence
analysis by graphs
AU Benight, Albert S.; Pancoska, Petr; Owczarzy, Richard;
Vallone, Peter M.; Nesetril, Jaroslav; Riccelli, Peter V.
CS Department of Chemistry, University of Illinois, Chicago, IL,
60607, USA
SO Methods in Enzymology (2001), 340(Drug-Nucleic Acid
Interactions), 165-192 CODEN: MENZAU; ISSN: 0076-6879
PB Academic Press
DT Journal; General Review
LA English

AB A review with refs. The anal. methods for characterizing DNA
sequence-dependent thermodn. stability have been reviewed. A
set of n-n sequence stability parameters is presented. Examples
in which these values are used to calc. the thermodn. stability of
short duplex DNA oligomers are presented. The problem of detg.
sets of isothermal sequences is addressed by representing DNA
sequences as graphs. Representing DNA sequences by a graph
descriptor with special math. properties minimizes the
computational difficulty of detg. the no. of DNA sequences with
identical predicted thermodn. stability. This is achieved by
replacement of a whole set of sequences by a single
representative. Applications of this concept were demonstrated
for sequences assembled from individual bases and sequences
assembled from oligomeric blocks. (c) 2001 Academic Press.
RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR
THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:746334 CAPLUS
DN 130:105911

TI Comparison of experimental to ***MELTSIM***
calculated ***DNA*** ***melting*** of the (A+T) rich
Dictyostelium discoideum genome: denaturation maps distinguish
exons from introns
AU Marx, Kenneth A.; Assil, Iman Q.; Bizzaro, J. W.; Blake, R. D.
CS Department of Chemistry, University of Massachusetts, Lowell,
MA, 01854, USA
SO Journal of Biomolecular Structure & Dynamics (1998), 16(2),
329-339 CODEN: JBSDD6; ISSN: 0739-1102

PB Adenine Press
DT Journal
LA English

AB The slime mold, Dictyostelium discoideum, possesses an (A+T) rich eukaryotic genome that is being sequenced in the Human Genome Project. High resoln. melting curves of isolated total and fractionated nuclear D. discoideum DNA (AX3 strain) were detd. exptl. and are compared to melting curves calcd. from GENBANK sequences (1.59% of genome) by the statistical thermodyn. program MELTSIM, parameterized for long DNA sequences. The lower and upper temp. limits of calcd. melting agree well with the obstd. melting of total DNA. The exptl. curve is unusual in that it contains a no. of sharp peaks. MELTSIM allowed us to calc. positional denaturation maps of D. discoideum GENBANK sequence documents contg. the 26S, 5.8S and 17S rDNA gene sequences, a major satellite DNA and repetitive sequence family present in 100-200 copies/nucleus. These denaturation maps contain subtransitions that correspond with a no. of the exptl. obstd. peaks, some of which we show to correspond with rDNA gene enriched CsCl gradient fractions of D. discoideum DNA. MELTSIM calcd. curves of coding, intron and flanking sequences indicate that both intron and flanking sequences are extremely (A+T) rich and account for most of the low temp. melting. There is no temp. overlap between thermal stabilities of these sequence domains and those of coding DNA. The latter must satisfy triplet codon constraints of higher (G+C) content. These large stability property differences enable a denaturation mapping feature of MELTSIM to clearly distinguish exon positions from those of introns and flanking DNA in long D. discoideum gene contg. sequences.

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:593023 CAPLUS
DN 129:299874

TI ***Melting*** of cross-linked ***DNA*** . III.
Calculation of differential ***melting*** curves
AU Lando, Dmitri Y.; Fridman, Alexander S.; Krot, Vladimir I.;
Akhrem, Afanasiia A.
CS Institute of Bioorganic Chemistry, Belarus National Academy
of Sciences, Minsk, 220141, Belarus
SO Journal of Biomolecular Structure & Dynamics (1998), 16(1),
59-67 CODEN: JBSDD6; ISSN: 0739-1102
PB Adenine Press
DT Journal
LA English
AB In our previous papers I and II (D. Y. Lando et al, J. Biomol. Struct. Dynam. (1997) v. 15, N1, p.129-140, p. 141-150), two methods were developed for calcn. of melting curves of cross-linked DNA. One of them is based on Poland's and another on the Fixman-Freire approach. In the present communication, III, a new theor. method is developed for computation of differential melting curves of DNAs cross-linked by anticancer drugs and their inactive analogs. As Poland's approach, the method allows study

of the influence of the loop entropy factor, $\delta(n)$, on melting behavior (n is the length of a loop in base pairs). However the method is much faster and requires computer time that inherent for the most rapid Fixman-Freire calcn. approach. In contrast to the computation procedures described before in communications I and II, the method is suitable for computation of differential melting curves in the case of long DNA chains, arbitrary loop entropy factors of melted regions and arbitrary degree of crosslinking including very low values that occur in vivo after administration of antitumor drugs. The method is also appropriate for DNAs without cross-links. The results of calcn. demonstrate that even very low degree of crosslinking alters the DNA differential melting curve. Crosslinking also markedly strengthens the influence of particular function $\delta(n)$ upon melting behavior.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:142910 CAPLUS
DN 118:142910

TI Modified self-consistent phonon ***calculation*** of the dependence of ***DNA*** ***melting*** temperature on guanine-cytosine content
AU Feng, Y.; Tan, S. C.
CS Dep. Phys., Natl. Univ. Singapore, Singapore, 0511, Singapore
SO Physical Review A: Atomic, Molecular, and Optical Physics (1992), 46(12), 8002-6 CODEN: PLRAAN; ISSN: 0556-2791

DT Journal
LA English

AB The self-consistent phonon approach was modified to treat DNA double helixes modeled with a large repeating unit (N base pairs) so that melting behaviors of DNA polymers of various base-pair sequences can be studied. The melting temps. of DNA polymers of different G-C-to-A-T ratios were calcd. (G, C, A, and T denote guanine, cytosine, adenine, and thymine, resp.). A DNA polymer with a relatively higher content of A-T melts at a lower temp. than DNA with a higher content of G-C. The melting temp. increases linearly when the G-C content in a DNA polymer increases. This is in agreement with both exptl. observations and theor. analyses.

L1 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:492436 CAPLUS
DN 111:92436

TI Long-range structural effects in supercoiled ***DNA*** : statistical thermodynamics reveals a correlation between ***calculated*** cooperative ***melting*** and contextual influence on cruciform extrusion
AU Schaeffer, Francis; Yeramian, Edouard; Lilley, David M. J.
CS Dep. Biol. Mol., Inst. Pasteur, Paris, 75724, Fr.
SO Biopolymers (1989), 28(8), 1449-73 CODEN: BIPMAA; ISSN: 0006-3525

DT Journal
LA English

AB C-type inducing sequences, which cause cruciform extrusion by adjacent inverted repeats were studied by applying statistical thermodyn. DNA helix melting theory. There was a marked correlation between the ability of sequences to confer C-type cruciform character exptl. and their calcd. propensity to undergo cooperative melting, and no exceptions were found. The correlations are both qual. and quant. Thus the ColE1 flanking sequences behave as single melting units, whereas the DNA of the S-type plasmid pIRbke8 exhibits no propensity to melt in the region of the bke cruciform. The results of the calcn.s. are also fully consistent with the following exptl. observations: (1) the ability of the isolated colL and ColR fragments of the ColE1

flanking sequences, as well as the short sequence col30, to confer C-type character; (2) C-type induction by an adenine- and thymine-rich Drosophila sequence; (3) low-temp. cruciform extrusion by an (AT)34 sequence; (3) low-temp. cruciform extrusion by an (AT)34 sequence; (4) the effect of changing sequences at a site 90 base pairs removed from the inverted repeat; (5) the effects of systematic deletion of the colL sequence; and (6) the effects of insertion of various sequences in between the colL sequence and the xke inverted repeat. Telestability effects on thermal denaturation as predicted from equil. helix melting theory of linear DNA may explain all the features that are revealed by studying the extrusion of cruciforms in circular DNA subjected to superhelical stress.

L1 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:149988 CAPLUS
DN 110:149988

TI ***Calculated*** ***melting*** temperature of methylated Z- ***DNA***

AU Hua, X.; Feng, Y.; Prohofsky, E. W.
CS Dep. Phys., Purdue Univ., Lafayette, IN, USA
SO Report (1988), Order No. AD-A193115, 22 pp. Avail.: NTIS

From: Gov. Rep. Announce. Index (U. S.) 1988, 88(18), Abstr. No. 847,050

DT Report

LA English

AB There are 2 approaches to theor. calcn. of DNA melting temp. One is based on a 2 states, quasi-1-dimensional lattice model in which the melting profile and differentiated melting curve could be calcd. as a function of DNA length. Another way is the modified self-consistent effective phonon approxn. (MSPA) in which the dynamic motional behavior of the DNA mol. during the melting process is detailed. The later approach to melting of methylated Z-DNA was used and results were compared to a similar calcn. on unmethylated B-DNA. A calcn. of melting temp. of methylated Z-DNA based on MSPA was presented.

L1 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:420072 CAPLUS
DN 101:20072

TI ***Calculator*** -controlled high resolution ***melting*** measurements of bacterial ***DNAs*** ; basic information for taxonomy studies. (Proposal and reality)

AU Pivec, L.; Vitek, A.; Rozkot, F.; Formanek, P.; Tille, D.; Felsberg, J.; Prauser, H.
CS Inst. Mol. Genet., Czech. Acad. Sci., Prague, Czech.
SO Colloque INSERM (1983), 114(Bacillus Gram Negat. Interet Med. Sante Publique), 39-47 CODEN: CINMDE; ISSN: 0768-3154

DT Journal

LA English

AB The absorption melting profiles of DNAs from various bacterial species were detd. by using a spectrophotometer connected to a computer, and the melting curves were used for calcg. phylogenetic relations among bacteria by using various methods (e.g., the function distance and the genetic distance methods, and computer tomog.). DNA from each bacterial strain showed a specific melting profile. None of the methods used for detg. phylogenetic relations provided full correlation with DNA hybridization results (although the function distance method showed the best correlation). A single absorption melting curve did not provide sufficient information for the anal. of the melting substructure.

L1 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:599242 CAPLUS
DN 95:199242

TI Effect of selectively-binding ligands on ***DNA*** helix-coil transition. III. ***Calculation*** of the ***melting*** curve of ***DNA*** -ligand complexes

AU Akhrem, A. A.; Lando, D. Yu.

CS Inst. Bioorg. Chem., Minsk, USSR

SO Molekulyarnaya Biologiya (Moscow) (1981), 15(5), 1083-92

CODEN: MOBIBO; ISSN: 0026-8984

DT Journal

LA Russian

AB DNA with a low degree of heterogeneity (synthetic periodic heteropolynucleotides and satellite DNA) exhibited little change in the temp. interval of melting in the presence of increasing concns. of selectively (guanine-cytosine) and nonselectively binding destabilizing and stabilizing ligands. DNA with a high degree of heterogeneity (the major part of DNA of higher organisms) exhibited a broadening of the temp. interval of melting and an increase (or decrease) in the melting temp. in the presence of increasing concns. of selectively binding stabilizing (or destabilizing) ligands. Nonselectively binding ligands at increasing concns. had little effect on melting temp. and a modest effect on the temp. interval of melting. There is apparently a change in the adenine-thymine:guanine-cytosine ratio in helical and melted segments of high-heterogeneity DNA as denaturation proceeds, and the availability of new ligand binding sites results in broadening of the melting temp. range. This ratio does not change in DNA of low heterogeneity.

L1 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:204033 CAPLUS
DN 94:204033

TI Stabilities of nearest-neighbor doublets in double-helical ***DNA*** determined by fitting ***calculated*** ***melting*** profiles to observed profiles

AU Gotoh, Osamu; Tagashira, Yusaku

CS Dep. Biochem., Saitama Cancer Cent. Res. Inst., Saitama, 362, Japan

SO Biopolymers (1981), 20(5), 1033-42 CODEN: BIPMAA; ISSN: 0006-3525

DT Journal

LA English

AB Melting profiles were calcd. for restriction fragments of λ -phage and fd phage DNAs and compared with exptl. profiles. The algorithm of M. Fixman and J.J. Freire (1977) was slightly modified so that a stability parameter was assigned not to a base pair but to each nearest-neighbor doublet. Stabilities of the 10 kinds of nearest-neighbor doublets were estd. by fitting the calcd. profiles to the obsd. ones. Agreement of the calcd. and obsd. profiles was much improved by this modification. The most interesting finding was that purine (3'-5') pyrimidine stackings are much more stable than their resp. reverses. The order of nearest-neighbor stabilities is in excellent agreement with that of neg. stacking energies calcd. by R. Rein and coworkers (1973) by a quantum-chem. method.

L1 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:82692 CAPLUS
DN 86:82692

TI The disordered Ising chain: Equivalent formulations for the thermodynamics

AU Chalupa, J.; Grinstein, G.; Wortis, Michael

CS Dep. Phys., Univ. Illinois, Urbana, IL, USA

SO Journal of Chemical Physics (1976), 65(11), 4512-14 CODEN: JCPSA6; ISSN: 0021-9606

DT Journal

LA English

AB For a 1-dimensional spin-(1/2) Ising model in which the exchange constant between each neighboring pair of spins and

the magnetic field at each spin site are random variables, the free energy can be expressed in terms of the soln. to a homogeneous integral equation derived by A. A. Vedenov and A. M. Dykhne (1968) and C. Fan and B. M. McCoy (1969). In using this model to ***calculate*** the ***melting*** curve of ***DNA***, G. W. Lehman and J. P. McTague (1968) gave 2 equiv. inhomogeneous equations that determine the free energy. These formalisms are shown to be equiv. by transforming the homogeneous equation into the inhomogeneous equations. A formal representation of the free energy as an infinite continued fraction is given.

L1 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:503008 CAPLUS
DN 69:103008

TI ***Calculation*** of ***melting*** curves for ***DNA***
AU Crothers, Donald M.
CS Yale Univ., New Haven, CT, USA
SO Biopolymers (1968), 6(10), 1391-404 CODEN: BIPMAA; ISSN:
0006-3525
DT Journal
LA English

AB A method is reported for calcg. the melting curve of a DNA mol. of random base sequence, including in the calcs. the dependence of the free energy of base pair formation on the size of a denatured section. Particular attention is drawn to the variation of local melting behavior from one region of the mol. to another. Sections rich in AT melt at relatively low temps. with a fairly broad transition curve, whereas regions rich in GC pairs melt at higher temps. with a very abrupt local transition curve. To account qual. for the results, one may divide melting into two kinds of processes: (a) the nucleation and growth of denatured regions, and (b) the merging together of two denatured sections at the expense of the intervening helix. The first of these processes dominates in the first stages of melting, and leads to rather broad local melting curves. The second process predominates in the later stages, and occurs, in a particular part of the mol., over a very narrow temp. range. It is estd. that the av. length of a helix plus adjacent coil section at the midpoint of the transition is approx. 600 base pairs. Since transition curves which measure the local melting behavior reflect local compn. fluctuations, these curves contain information about the broad outlines of base sequence in the mol. Some suggestions are made concerning experiments by which this potential informations source could be exploited. Thus, one might map AT- or GC-rich regions at particular genetic loci in a biol. active DNA mol. Values of the relevant parameters found earlier for the transition of homopolymers produce melting curves for a DNA of random base sequence which are in good agreement with the exptl. transition curve for T2 phage DNA. Therefore, the present theoretical picture of the melting of polynucleotides is at least internally self-consistent.

L1 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:400092 CAPLUS
DN 69:92

TI A semiempirical analysis of the ***melting*** curves of synthetic ***DNA*** molecules and the ***calculation*** of the stacking and pairing energies and entropies in DNA
AU Goel, Narendra S.; Fukuda, Nobuo; Rein, Robert
CS Univ. of Rochester, Rochester, NY, USA
SO Journal of Theoretical Biology (1968), 18(3), 350-70 CODEN:
JTBIA; ISSN: 0022-5193

DT Journal
LA English
AB A semi-empirical anal. of the available exptl. data on the melting temps. and widths of the melting curves of various

synthetic DNAs was made using a modified Ising model with the nearest-neighbor interactions only, and values for the entropies of denaturation, A-T and G-C bonds energies, and stacking energies for the various nearest-neighbor base pairs were calcd. These values fell within a chem. reasonable range, suggesting that the modified Ising model with nearest-neighbor interactions only, is internally consistent, and satisfactorily describes the melting phenomenon. 30 references.

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